

# NON-LINEAR FINITE ELEMENT MODELLING OF LIGHT-TO-HEAT ENERGY CONVERSION APPLIED TO NANOENCAPSULATED PHASE CHANGE MATERIALS

JOSEP FORNER-ESCRIG\*<sup>†</sup>, ROSA MONDRAGÓN<sup>†</sup> and ROBERTO  
PALMA<sup>†</sup>

\*<sup>†</sup> Department of Mechanical Engineering and Construction  
Universitat Jaume I (UJI)  
Av. de Vicent Sos Baynat, s/n 12071 Castelló de la Plana, Spain  
e-mail: jforner@uji.es

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**Abstract.** In nature, physical phenomena tend to exhibit their effects simultaneously and, depending on the situation of study, their interactions cannot be neglected. For instance, nanofluids, which are composed of both fluid and nanosolids, are currently used for thermal energy storage in concentrated solar power plants and couple thermal and mechanical fields. Notice that owing to some limitations of solar collectors, fluids combined with nanoparticles are under research currently to absorb solar energy by light-to-heat conversion of energy. On this ground, the aim of the present work is to develop a numerical formulation within the finite element method (FEM) to study the light-to-heat energy conversion, phase-change and thermal stresses in nanosolids. For this purpose and in a first and good approximation, it is assumed that the light is converted into heat by the Joule heating —a non-linear term which quadratically depends on the electric field. Therefore, the set of three coupled governing equations is composed of: balance of linear momentum for the mechanical field, balance of energy for the thermal field and balance of electric current for the electric field. These equations are rewritten in a weak form, which is more amenable in the context of the FEM, and they are implemented in a numerical code. Finally, several benchmarks are presented to validate the numerical results against analytical solutions developed by the authors.

## 1 INTRODUCTION

The rapid development of societies nowadays increases more and more the consumption of energy around the world. In order to fight against the consequences of climate change, renewable energies are growing in importance. Among the different types of renewable

energies, solar energy and more specifically solar thermal energy are of special interest [1]. A main application of solar thermal energy is concentrated solar power (CSP) plants [2], where phase change materials (PCMs) are combined with heat transfer fluids (HTF) to enhance both sensible and latent energy storage. In order to improve the efficiency of these systems, the addition of nanoencapsulated phase change materials (nePCMs) is currently under research [3, 4]. The combination of nanoparticles with a fluid is known as nanofluid [5].

Due to the limitations that solar collectors present such as corrosion, considerable heat losses and limitations on the incident flux, fluids mixed with nanoparticles are under research instead to absorb directly the solar energy [6]. This combination of liquids with nanoparticles is also known as solar nanofluids [7].

Currently, to the best of the author's knowledge, a solar nanofluid containing nePCMs has not been attempted by the experimental community due to the fact that the increase in temperature achieved by solar radiation is not sufficient to melt the core of nePCMs. However, the aim of this work is to provide a general numerical framework to analyse the behaviour of a generic nanoparticle by including thermomechanical phase change with light-to-heat conversion. In particular, this work presents a numerical formulation within the finite element (FE) method [8]. Previously, a consistent thermodynamic approach is performed to obtain the set of three-dimensional governing equations. Then, these equations are discretised by following FE standard procedures and implemented in the research code **FEAP** [9], which belongs to the University of California at Berkeley (USA). In order to validate the code, numerical solutions are compared with analytical ones developed by the authors.

Table 1 summarizes the mathematical notation used through the present work.

## 2 GOVERNING EQUATIONS

Three coupled partial differential equations are required to describe light-to-heat conversion in nePCMs. These equations are often called governing equations and are composed of balance equations and of boundary conditions.

### 2.1 Balance equations

Consider a general domain of study  $\Omega$ , boundary  $\partial\Omega$  and outward normal  $\underline{n}$  containing solid and liquid phases. Four balance equations must be considered: linear and angular momentum balances, energy balance and electric charge balance for the whole domain.

#### 2.1.1 Mechanical balance

The strong form of the linear momentum balance reads:

$$\rho \ddot{\underline{u}} = \nabla \cdot \underline{\underline{\sigma}} + \underline{f} \quad (1)$$

Table 1: Notation.

Mathematical operators	Description
$\dot{()}$	First time derivative
$\ddot{()}$	Second time derivative
$\underline{()}$	First order tensor
$\underline{\underline{()}}$	Second order tensor
$\underline{\underline{\underline{()}}}$	Fourth order tensor
$()^\top$	Transpose
$\text{tr}()$	Trace
$() \cdot ()$	Dot product
$() : ()$	Double contraction product
$() \otimes ()$	Tensor product

where  $\rho, \ddot{\underline{u}}, \underline{\underline{\sigma}}, \underline{f}$  denote mass density, acceleration, Cauchy stress tensor and body force vector, respectively. The stress tensor is related to the traction vector  $\underline{t}$  by the Cauchy relation:  $\underline{t} = \underline{\underline{\sigma}} \cdot \underline{n}$ . The Cartesian components of the displacement vector are defined as  $\underline{u} = (u, v, w)$ .

Secondly, the angular momentum balance is automatically satisfied by the symmetry of the Cauchy stress tensor:  $\underline{\underline{\sigma}} = \underline{\underline{\sigma}}^\top$ .

### 2.1.2 Energy balance

The energy balance is written in the present work in terms of enthalpy, which is defined as:

$$H = \int_{T_{ref}}^T \rho c \, d\theta + \rho L h(T - T_m) \quad (2)$$

where  $c, L$  denote heat capacity and latent heat, respectively. The variable  $T$  represents temperature and  $T_{ref}$  and  $T_m$  denote reference temperature at which enthalpy is calculated and melting temperature, respectively. Finally,  $h(T - T_m)$  is the Heaviside step function, which is defined as follows:

$$h(T - T_m) = \begin{cases} 0 & \text{if } T < T_m \\ 1 & \text{if } T > T_m \end{cases} \quad (3)$$

According to the previous definitions, the local form of eq. (2) becomes:

$$\frac{dH}{dt} + \underline{\nabla} H \cdot \underline{\dot{u}} = -\underline{\nabla} \cdot \underline{q} + \underline{j} \cdot \underline{E} \quad (4)$$

where  $\underline{\dot{u}}$ ,  $\underline{q}$ ,  $\underline{j}$  and  $\underline{E}$  denote velocity, heat flux vector, electric flux vector and electric field, respectively. The last term in eq. (4) represents the contribution of Joule heating.

Notice that the phase change problem considered within the energy balance in the present work is that of pure substances. More specifically, the algorithm used in the present work to solve phase change numerically is the enthalpy method reported in [10].

### 2.1.3 Electric charge balance

The strong form of the electric charge balance may be expressed as:

$$\frac{d\rho_q^f}{dt} = -\underline{\nabla} \cdot \underline{j} \quad (5)$$

where  $\rho_q^f$  denotes the free electric charge.

Notice that a source/sink term does not exist in eq. (5) due to the fact that electric charge is neither created nor destroyed [11].

## 2.2 Constitutive equations

Constitutive equations describe the behaviour of the media contained in the domain of study.

### 2.2.1 Thermomechanical constitution

The constitutive equation of the solid phase that relates strain, temperature and stress is:

$$\underline{\underline{\sigma}}_s = \underline{\underline{C}} : \underline{\underline{\varepsilon}} - \underline{\underline{\beta}} (T - T_{ref}) \quad (6)$$

where  $\underline{\underline{C}}$ ,  $\underline{\underline{\varepsilon}}$  and  $\underline{\underline{\beta}}$  denote the fourth-order elastic tensor, the infinitesimal strain tensor and the second order thermoelastic tensor, respectively.

Tensors  $\underline{\underline{C}}$  and  $\underline{\underline{\beta}}$  are defined as follows:

$$\begin{aligned} \underline{\underline{C}} &= \lambda \underline{\underline{I}} \otimes \underline{\underline{I}} + 2\mu \underline{\underline{I}}^{sy} \\ \underline{\underline{\beta}} &= (3\lambda + 2\mu) \alpha \underline{\underline{I}} \end{aligned} \quad (7)$$

where  $\underline{\underline{I}}$ ,  $\underline{\underline{I}}^{sy}$  denote second and symmetric part fourth order identity tensors, respectively [12]. In turn,  $\alpha$ ,  $\lambda$  and  $\mu$  denote the coefficient of thermal expansion and Lamé parameters, respectively. Lamé parameters are defined as:

$$\lambda = \frac{E\nu}{(1+\nu)(1-2\nu)}, \quad \mu = \frac{E}{2(1+\nu)} \quad (8)$$

where  $E$  and  $\nu$  represent Young's modulus and Poisson's ratio, respectively.

The constitutive equation for a static fluid phase is:

$$\underline{\underline{\sigma}}_l = p \underline{\underline{I}} \quad (9)$$

where  $p$  is the thermodynamic pressure of the fluid. In the present work, as an approximation, the liquid phase is assimilated to a fluid at rest given that the liquid volume inside the nanoparticles (at the order of nanometers) is reduced and consequently, dynamic effects can be neglected. Therefore, the pressure in the fluid can be computed as the spherical part of the stress tensor in the solid phase:

$$p = \frac{1}{3} \text{tr}(\underline{\underline{\sigma}}_s) \quad (10)$$

### 2.2.2 Heat conduction

The relation between heat flux and temperature is:

$$\underline{q} = -\underline{\underline{\kappa}} \cdot \underline{\nabla} T \quad (11)$$

where  $\underline{\underline{\kappa}}$  denotes the thermal conductivity tensor.

### 2.2.3 Electricity conduction

The relation between electric flux and electric field is:

$$\underline{j} = \underline{\underline{\gamma}} \cdot \underline{E} \quad (12)$$

where  $\underline{\underline{\gamma}}$  denotes the electric conductivity tensor.

## 2.3 Boundary conditions

The boundary conditions are composed of Dirichlet (also known as first-type) or Neumann (second-type) expressions:

$$\begin{array}{llll} \text{Dirichlet} & \underline{u} = \underline{\bar{u}} & T = \bar{T} & V = \bar{V} \\ \text{Neumann} & \underline{\underline{\sigma}} \cdot \underline{n} = \underline{\bar{t}} & \underline{q} \cdot \underline{n} = \bar{q} & \underline{j} \cdot \underline{n} = \bar{j} \end{array} \quad (13)$$

where  $\underline{\bar{u}}$ ,  $\bar{T}$ ,  $\underline{\bar{t}}$ ,  $\bar{q}$ ,  $\bar{V}$  and  $\bar{j}$  are the prescribed displacements, temperature, traction, thermal flux, voltage and electric flux, respectively. The variable  $V$  represents voltage.

Finally, these governing equations are written in weak forms and discretised to be implemented in the numerical code **FEAP**.

### 3 NUMERICAL BENCHMARKS

In this section, several validations of the formulation are performed by comparing numerical and analytical solutions developed by the authors. For the validations, it is assumed that the variation of free electric charge with time is negligible. Material properties of tin (Sn) are considered; see [10] for further detail.

Two different cases are studied to validate the numerical implementation. In case I, a thermomechanical problem with phase change is defined while in case II, a steady state problem of electro-thermoelasticity without phase change is the object of study.

#### 3.1 Case I

An analytical solution is developed for a one-dimensional half-space domain, with a time-dependent temperature prescribed at its free end. The domain is traction free. More detail about the analytical solution is given in [10].

In this case, for the validations, prescribed and initial temperatures are respectively:  $T_0 = 583$  K (above melting temperature  $T_m = 504.95$  K),  $T_i = 323$  K.

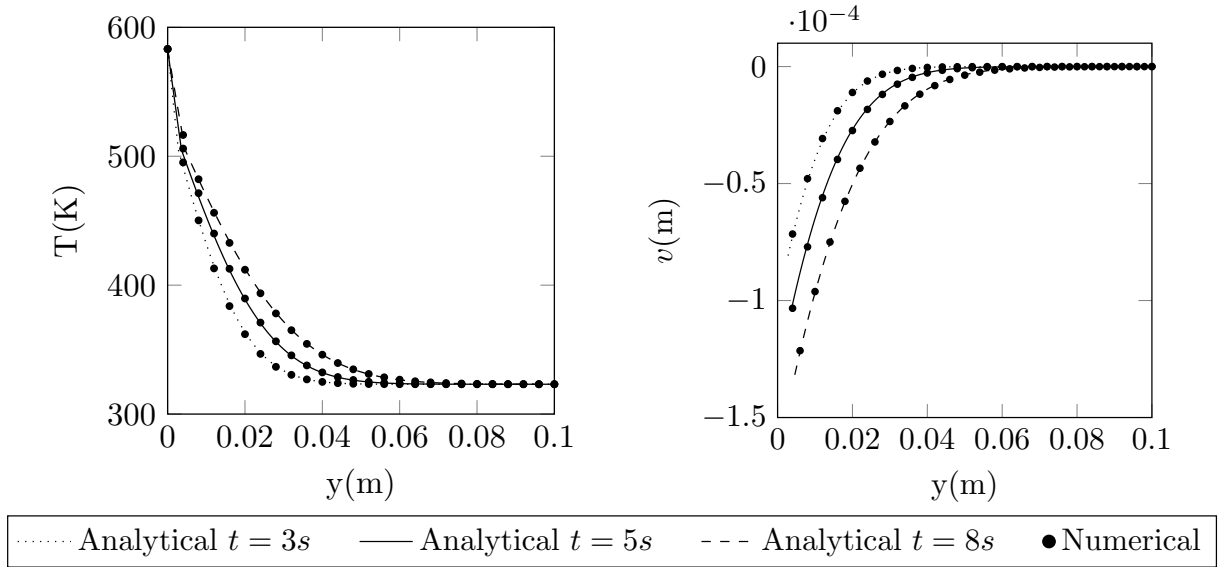


Figure 1: Comparison of analytical and numerical temperature distributions (left) and axial displacement (right) for three different times along the one-dimensional geometry.

For these numerical simulations, 200 elements are used. Eight-noded brick elements with standard shape functions of Lagrange-type are used to interpolate the results. The maximum relative error is lower than 1% between analytical and numerical solutions of temperature and lower than 4% between those of displacement. Notice that the validation of the axial displacement in Figure 1 is only done for the solid phase.

### 3.2 Case II

An analytical solution is developed for a one-dimensional body for a steady state study. In this case, voltage and temperature values (below the melting temperature  $T_m = 504.95$  K) are prescribed at both ends of the one-dimensional geometry. The body is traction free and one of the ends is mechanically fixed ( $v_1 = 0$ ).

In this case, for the validations, prescribed values of temperature and voltage are respectively:  $T_1 = 303$  K,  $T_2 = 353$  K,  $V_1 = 0$  V,  $V_2 = 0.1$  V. Subscripts 1 and 2 refer to left and right ends of the one-dimensional geometry, respectively.

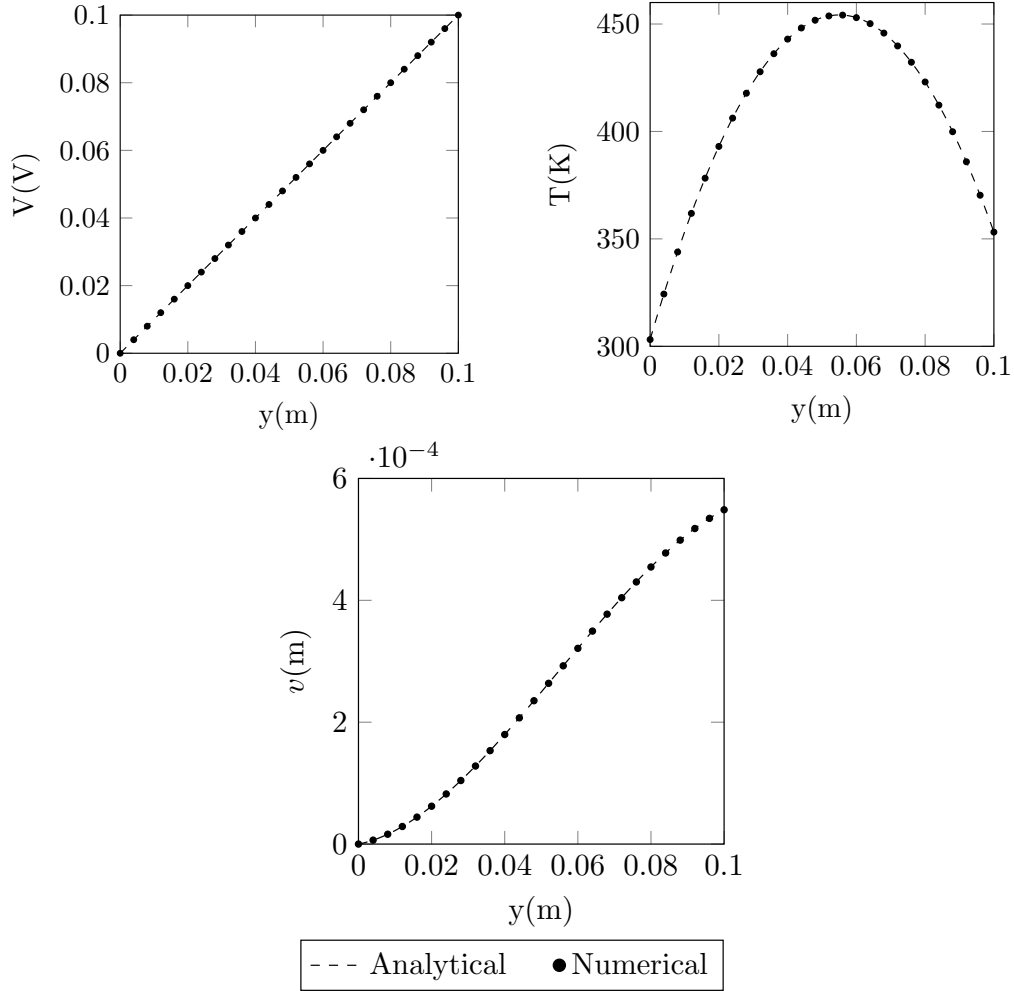


Figure 2: Comparison of analytical and numerical voltage distribution (left, upper row), temperature distribution (right, upper row) and axial displacement (lower row) along the one-dimensional geometry.

For these numerical simulations, 200 elements are used. Eight-noded brick elements with standard shape functions of Lagrange-type are used to interpolate the results. The maximum relative error is lower than 0.1% between analytical and numerical solutions for the three magnitudes shown in Figure 2.

## 4 CONCLUSIONS

In this work, a FE formulation is proposed to deal with thermoelasticity with light-to-heat energy conversion. By comparing numerical and analytical solutions, it can be observed that a good agreement exists between both results. Therefore, the numerical model is validated and could be a useful tool to conduct multiphysics numerical analysis or predicting the stresses developed in nePCMs.

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## REFERENCES

- [1] G. Xiao, K. Guo, Z. Luo, M. Ni, Y. Zhang, and C. Wang, “Simulation and experimental study on a spiral solid particle solar receiver,” *Applied Energy*, vol. 113, pp. 178 – 188, 2014.
- [2] N. Bozorgan and M. Shafahi, “Performance evaluation of nanofluids in solar energy: a review of the recent literature,” *Micro and Nano Systems Letters*, vol. 3, p. 5, 2015.
- [3] N. Navarrete, A. Gimeno-Furió, R. Mondragón, L. Hernández, L. Cabedo, E. Cordocillo, and J. E. Juliá, “Nanofluid based on self-nanoencapsulated metal/metal alloys phase change materials with tuneable crystallisation temperature,” *Scientific Reports*, vol. 7, 2017.
- [4] N. Navarrete, R. Mondragón, D. Wen, M. E. Navarro, Y. Ding, and J. E. Juliá, “Thermal energy storage of molten salt based nanofluid containing nano-encapsulated metal alloy phase change materials,” *Energy*, vol. 167, pp. 912 – 920, 2019.
- [5] S. Choi and J. Eastman, “Enhancing thermal conductivity of fluids with nanoparticles,” *Proceedings of the ASME International Mechanical Engineering Congress and Exposition, San Francisco, CA, USA*, 1995.



- [6] K. Khanafer and K. Vafai, “A review on the applications of nanofluids in solar energy field,” *Renewable Energy*, vol. 123, pp. 398 – 406, 2018.
- [7] T. P. Otanicar and J. S. Golden, “Comparative environmental and economic analysis of conventional and nanofluid solar hot water technologies,” *Environmental Science & Technology*, vol. 43, pp. 6082 – 6087, 2009.
- [8] O. Zienkiewicz and R. Taylor, *The Finite Element Method 7th Edition*. Butterworth-Heinemann, 2013.
- [9] R. Taylor, *FEAP A Finite Element Analysis Program: User Manual*. University of California, Berkeley, 2013. <http://www.ce.berkeley.edu/feap>.
- [10] J. Forner-Escrig, R. Mondragón, and R. Palma, “Finite element formulation to investigate thermomechanical behaviour in nanoencapsulated phase change materials for energy storage,” *Submitted for publication*, 2019.
- [11] R. Palma, E. Moliner, and J. Forner-Escrig, “Computational thermoelectricity applied to cooling devices,” in *Bringing Thermoelectricity into Reality* (P. Aranguren, ed.), ch. 13, IntechOpen, 2018. Open access. Available at: <https://www.intechopen.com/books/bringing-thermoelectricity-into-reality/computational-thermoelectricity-applied-to-cooling-devices>.
- [12] E. W. V. Chaves, *Mecánica del Medio Continuo. Conceptos básicos-3 Edición*. CIMNE, 2012.